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K. T. Cheng, M. H. Chen

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A large-scale relativistic configuration-interaction calculation for the $4s - 4p$ and $4p - 4d$ transition energies of Copperlike heavy ions ⋆

K. T. Cheng and M. H. Chen

Lawrence Livermore National Laboratory, Livermore, CA 94550 USA

Abstract

The $4s - 4p$ and $4p - 4d$ transition energies for high-Z copperlike ions are calculated using the relativistic configuration-interaction (RCI) method. Mass polarization (MP) and quantum electrodynamic (QED) corrections are also evaluated. For the $4s - 4p$ transitions, the present RCI energies agree very well with results from the relativistic many-body perturbation theory. With QED and MP corrections included, our total transition energies are in very good agreement with recent high precision measurements.

Key words: Atomic spectroscopy, QED corrections
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The spectra of Cu-like ions feature prominent resonance lines from the $4s - 4p$ and $4p - 4d$ transitions. Recent high-precision measurements [1–4] of these lines in high-Z Cu-like ions have achieved accuracies down to a few tens of meV. They provide stringent tests of relativistic correlation calculations as well as quantum electrodynamic (QED) theory in the presence of strong external fields. To compare with these experiments, we have carried out large-scale relativisitc configuration-interaction (RCI) calculations for the $4s - 4p$ and $4p - 4d$ transition energies in high-Z Cu-like ions.

Details of our RCI method can be found in Ref. [5] and references therein. Briefly, our RCI calculations are based on the relativistic no-pair Hamiltonian

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Table 1
Contributions to the $4s-4p$ and $4p-4d$ transition energies (eV) of Cu-like uranium.

Term	$4s-4p_{1/2}$	$4s-4p_{3/2}$	$4p_{1/2}-4d_{3/2}$	$4p_{3/2}-4d_{3/2}$	$4p_{3/2}-4d_{5/2}$
Coulomb	146.76	473.15	539.94	213.52	281.03
Breit	2.70	-0.85	-4.10	-0.55	-1.76
RCI	149.46(2)	472.30(2)	535.84(2)	212.97(2)	279.27(2)
MP	0.00	0.00	-0.09	-0.09	-0.09
Self-energy	-4.24	-4.33	-0.88	-0.79	-0.65
Uehling	1.02	1.25	0.24	0.01	0.01
WK	-0.05	-0.06	-0.02	0.00	0.00
Relax	-0.02	0.03	0.08	0.03	0.04
2-loop	0.02	0.02	0.00	0.00	0.00
QED	-3.27(5)	-3.09(5)	-0.58(5)	-0.76(5)	-0.60(5)
Total	146.19(5)	469.21(5)	537.17(5)	212.12(5)	278.59(5)

which includes the Coulomb and frequency-dependent, retarded Breit interactions. Positive-energy projection operators are used in the no-pair Hamiltonian to prevent spurious interactions with virtual electron-positron pairs. Many-electron configuration-state functions (CSF) are constructed from one-electron B-spline, or basis spline, functions which are radial Dirac orbits of an electron moving in a screened nuclear potential confined to a finite cavity. B-spline orbitals form a complete, finite basis set and separate cleanly into positive- and negative-energy states. The no-pair requirement is implicitly satisfied by using only positive-energy B-spline orbitals in our RCI calculations. All single- and double-excitations from core-valence and core-core interactions are systematically included for well converged RCI energies. Resulting large-scale RCI expansions reach over 300,000 configurations and Davidson's method is used to solve for the first few eigenstates of these big RCI matrices. Mass polarization (MP) corrections are then calculated as expectation values of the operator $(1/M)\Sigma_{i>j}\,\mathbf{p}_i \cdot \mathbf{p}_j$ using RCI wave functions.

In this work, QED energies are calculated from the one-loop self-energy and vacuum polarization corrections. Leading vacuum polarization corrections are evaluated as expectation values of the Uehling potential. Electron self-energies and Wichmann-Kroll (WK) corrections to the vacuum polarization are calculated non-perturbatively to all orders in $Z\alpha$ with partial wave expansions of electron Green's functions. To account for screening and relaxation corrections, QED energies are evaluated in Dirac-Kohn-Sham (DKS) potentials specific to the initial and final states. Two-loop Lamb shift contributions are small and are estimated using scaling laws.

Table 2
$4s - 4p$ transition energies (eV) of Cu-like ions.

Contribution	W^{45+}	Au^{50+}	Pb^{53+}	Th^{61+}	U^{63+}
			$4s - 4p_{1/2}$		
Coulomb	97.85	110.49	118.43	140.85	146.76
RMBPT [6]	97.83	110.47	118.40	140.83	146.74
Breit	1.05	1.40	1.64	2.46	2.70
RMBPT [6]	1.06	1.40	1.65	2.47	2.72
QED	-1.36	-1.78	-2.07	-3.00	-3.27
Blundell [7]	-1.34		-2.05	-2.98	-3.25
Kim *et al.* [8]	-1.33	-1.74	-2.02	-2.92	-3.18
Total	97.54	110.11	118.00	140.31	146.19
Expt-a [4]			118.010(1)		
Expt-b [9]	97.63(1)	110.22(1)	118.15(2)		146.39(37)
			$4s - 4p_{3/2}$		
Coulomb	200.26	255.25	294.78	430.73	473.15
RMBPT [6]	200.25	255.22	294.76	430.72	473.13
Breit	-0.13	-0.24	-0.33	-0.70	-0.85
RMBPT [6]	-0.14	-0.24	-0.33	-0.72	-0.86
QED	-1.24	-1.63	-1.91	-2.82	-3.09
Blundell [7]	-1.22		-1.88	-2.78	-3.05
Kim *et al.* [8]	-1.21	-1.59	-1.86	-2.73	-2.99
Total	198.89	253.38	292.54	427.21	469.21
EBIT-1 [1]	198.90(1)	253.40(1)	292.60(4)	427.20(4)	469.06(3)
EBIT-2 [2]				427.20(1)	469.22(3)
Expt-b [9]	198.99(5)	253.40(8)	292.65(10)	427.68(22)	469.53(25)

Table 1 shows various contributions to the $4s - 4p$ and $4p - 4d$ transition energies (eV) using Cu-like uranium as an example. It can be seen that mass polarization corrections are negligible for the $4s - 4p$ transitions but are quite sizeable for the $4p - 4d$ transitions. Also, while QED corrections for the $4p - 4d$ transitions are small at -0.6 to -0.8 eV, they are still significantly larger than the uncertainties of recent EBIT measurements [3]. Theoretical uncertainties quoted here are estimates only. For QED energies, they are due mainly to the approximated treatment of screening corrections.

Table 3
$4p_{1/2} - 4d_{3/2}$ transition energies (eV) of Cu-like ions.

Contribution	W^{45+}	Au^{50+}	Bi^{54+}	Th^{61+}	U^{63+}
Coulomb	253. 70	312. 88	369. 91	496. 27	539. 94
Breit	-1. 59	-2. 09	-2. 59	-3. 71	-4. 10
MP	-0. 04	-0. 05	-0. 06	-0. 08	-0. 09
QED	-0. 11	-0. 18	-0. 27	-0. 49	-0. 58
Total	251. 97	310. 56	367. 00	491. 99	535. 17
EBIT-3 [3]			366. 97(2)	491. 94(10)	535. 15(5)

Tables 2 and 3 show $4s - 4p$ and $4p_{1/2} - 4d_{3/2}$ transition energies for high-Z Cu-like ions. Our RCI energies agree with those of the relativistic many-body perturbation theory (RMBPT) [6]. Our QED energies agree with Blundell's results [7] but deviate from those obtained with Welton's method by Kim *et al.* [8]. Our $4s - 4p_{1/2}$ transition energy in Pb^{53+} is in excellent agreement with the recent dielectronic recombination measurement [4]. Our $4s - 4p_{3/2}$ and $4p_{1/2} - 4d_{3/2}$ transition energies are in excellent agreement with recent EBIT measurements [1–3]. It is also clear that early laser-plasma measurements of Seely *et al.* [9] are consistently too high in energy. In conclusion, we have shown that large-scale RCI calculations can get very accurate relativistic correlation energies for Cu-like ions. We have also shown that screening and relaxation corrections to the QED energies can be well approximated by evaluating self-energy and vacuum polarization contributions in DKS potentials.

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